checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_tca_br_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: cu_tca_br_0m

Bond precision: C-C = 0.0069 A   Wavelength=1.54178

Cell: a=20.9699(4)   b=20.9699(4)   c=20.9699(4)
                 alpha=90   beta=90   gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	9221.2(5)	9221.2(5)
Space group	I 2 3	I 2 3
Hall group	I 2 2 3	I 2 2 3
Moiety formula	2(C21 H15 N O6), 2(C21 H12 N O6), 2(C H Cl3), 3(H O), 6(H4 N)	2(C H Cl3), 2(C21 H15 N O6), 2(C21 H12 N O6), 6(H4 N), 1.5(H2 O
Sum formula	C86 H83 Cl6 N10 O27	C86 H83 Cl6 N10 O27
Mr	1901.32	1901.32
Dx,g cm-3	1.370	1.370
Z	4	4
Mu (mm-1)	2.393	2.393
F000	3948.0	3948.0
F000'	3969.03	
h,k,lmax		24,24,24
Nref		2462
Tmin,Tmax	0.488,0.512	0.580,0.752
Tmin'	0.443	

Correction method= # Reported T Limits: Tmin=0.580 Tmax=0.752
AbsCorr = NONE

Data completeness=   Theta(max)= 62.482

R(reflections)= 0.0522(2171)

wR2(reflections)=
0.1579(2462)

S = 1.103   Npar= 203

The following ALERTS were generated. Each ALERT has the format
      test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🟡 Alert level C

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STRVA01_ALERT_4_C          Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.500
          From the CIF: _refine_ls_abs_structure_Flack_su  24.000
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5752
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ    Please Check
          Calc: 2(C21 H15 N O6), 2(C21 H12 N O6), 2(C H Cl3), 3(H O), 6(H4 N
          Rep.: 2(C H Cl3), 2(C21 H15 N O6), 2(C21 H12 N O6), 6(H4 N), 1.5(H
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........    6.63 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....    3.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....    3.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl01    0.187 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    O00N    0.177 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.00686 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N006    --H00A    .   Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    3.197 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.73Ang From O00N   .   -0.55 eA-3
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement   Please Check
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      2 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............      5 Report
          H002  H00N  H00A  H00B  H00C
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .  0.500 Note
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large  0.11 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records     1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H00N    Constrained at      0.5 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D    H00C   ..H00N   .   1.62 Ang.
                              1/2+y,1/2-z,3/2-x =   23_556 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........   37 Note
          Cl01   O002   H002   O003   O004   O005   N006   H00A
          H00B   H00C   C007   N008   C009   C00A   N00B   C00C
          C00D   H00D   C00E   H00E   C00F   C00G   C00H   H00H
          C00I   H00I   C00J   H00J   C00K   H00K   C00L   H00L
          C00M   H00M   O00N   H00N   H00F
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #      2 Note
          C21 H12 N O6
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still   86% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).     1 Note
          0  1  1,
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .   0.34 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      0 Info
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   0 ALERT level A = Most likely a serious problem – resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_STRVA01_cu_tca_br_0m
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_THETM01_cu_tca_br_0m
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.590
RESPONSE: ...
;
_vrf_PLAT042_cu_tca_br_0m
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ    Please Check
RESPONSE: ...
;
_vrf_PLAT089_cu_tca_br_0m
;
PROBLEM: Poor Data / Parameter Ratio (Zmax < 18) ........     6.63 Note
RESPONSE: ...
;
_vrf_PLAT250_cu_tca_br_0m
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....     3.2 Note
RESPONSE: ...
;
_vrf_PLAT260_cu_tca_br_0m
;
PROBLEM: Large Average Ueq of Residue Including     Cl01     0.187 Check
RESPONSE: ...
;
_vrf_PLAT340_cu_tca_br_0m
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............   0.00686 Ang.
RESPONSE: ...
;
_vrf_PLAT420_cu_tca_br_0m
;
PROBLEM: D-H Bond Without Acceptor  N006     --H00A    .     Please Check
RESPONSE: ...
```

```
;
_vrf_PLAT906_cu_tca_br_0m
;
PROBLEM: Large K Value in the Analysis of Variance ......     3.197 Check
RESPONSE: ...
;
_vrf_PLAT976_cu_tca_br_0m
;
PROBLEM: Check Calcd Resid. Dens.  0.73Ang From O00N   .     -0.55 eA-3
RESPONSE: ...
;
_vrf_PLAT987_cu_tca_br_0m
;
PROBLEM: The Flack x is >> 0 -  Do a BASF/TWIN Refinement    Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock cu_tca_br_0m - ellipsoid plot